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SYNTHESIS OF NOVEL 1,2,3-THIADIAZOLES

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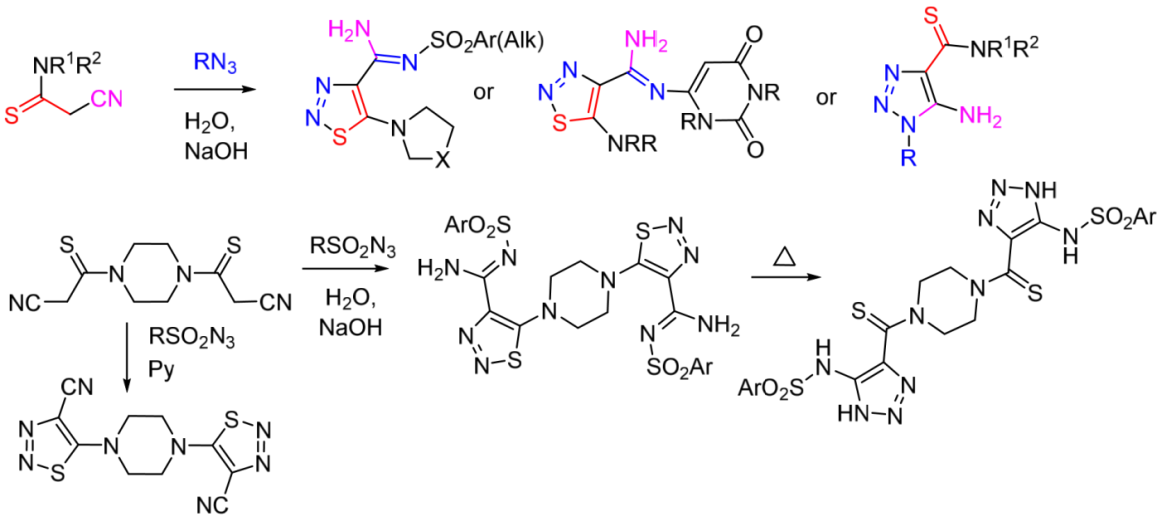
Abstract. The reactions of azides with thioamides in water were studied and it was shown that the reaction of 2-cyanothioacetamides with various types of azides in water in the presence of alkali presents an efficient, general, one-step, atom economic, eco-friendly method for the synthesis of 5-dialkylamino-1,2,3thiadiazol-4-carbimidamides and 1-aryl-5-amino-1,2,3-triazole-4-carbothioamides. This method can be extended to the one pot reaction of sulfonyl chlorides and 6-chloropyrimidine-2,4-diones with sodium azide leading to final products in higher yields, avoiding the isolation of unsafe sulfonyl azides. The method was furthermore applied to the reaction of *N*,*N*'-bis-(2-cyanothiocarbonyl)pyrazine with sulfonyl azides to afford bicyclic 1,2,3-thiadiazoles and 1,2,3-triazoles connected *via* a 1,1′-piperazinyl linker. 2Cyanothioacetamides were also shown to react with aromatic azides in water in the presence of alkali to afford 1-aryl-5-amino-1,2,3-triazole-4-carbothioamides. In contrast to aromatic azides and similarly to sulfonyl azides, 6-azidopyrimidine-2,4-diones react with cyanothioacetamides to form *N*-pyrimidin-6-yl5-dialkylamino-1,2,3-thiadiazole-4-*N*-l-carbimidamides. The role of water in changing the reactivity of azides towards 2-cyanothioacetamides was rationalized by a proposed mechanism.



References

1. Filimonov, V. O., Dianova, L. N., Galata, K. A., et al. (2017). A Switchable Synthesis of 4,5-Functionalized 1,2,3-Thiadiazoles and 1,2,3-Triazoles from 2Cyanothioacetamides under Diazo Group Transfer Conditions. *J. Org. Chem*., 82, Iss. 8, pp. 4056–4071.

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